1,5,7,11-Tetraoxaspiro[5.5]undecane
24472-02-4 | DTXSID1066994

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 23.8 days

Global applicability domain: Outside

Local applicability domain index: 2.17e-01

Confidence level: 7.22e-01

Nearest Neighbors from the Training Set

Image not found
Hexane, 2,2,5-trimethyl-
Measured: 777
Predicted: 17.4

Image not found
Pentane, 2,3,3-trimethyl-
Measured: 9340
Predicted: 23.3

Image not found
2,5-Dimethylhexane
Measured: 1650
Predicted: 23.8

Image not found
2,2,4-Trimethylpentane
Measured: 4890
Predicted: 30.5